

**To:** Hedrick, Elizabeth[Hedrick.Elizabeth@epa.gov]; Gray, Wendy[Gray.Wendy@epa.gov]; Arguto, William[Arguto.William@epa.gov]  
**Cc:** Sayles, Gregory[Sayles.Gregory@epa.gov]  
**From:** Weber, Eric  
**Sent:** Tue 2/4/2014 6:45:41 PM  
**Subject:** RE: MCHM & PPH Product TICs  
WV product information Weber 2-4-14.docx

Attached is the information I put together concerning the expected products in the storage tank based primarily on the MSDS sheets. Potential degradation products can also be added (see discussion below). Also, other pchem properties can be added as needed. I have included chemical structures to help address questions concerning potential isomers that might be present in the various products.

Eric

Eric J. Weber, Ph.D.

Research Chemist

Ecosystems Research Division

Office of Research & Development

U.S. Environmental Protection Agency

960 College Station Rd.

Athens, GA 30605

Phone: 706-355-8224

Email: weber.eric@epa.gov

**From:** Hedrick, Elizabeth  
**Sent:** Monday, February 03, 2014 12:23 PM  
**To:** Gray, Wendy; Weber, Eric; Arguto, William

**Cc:** Sayles, Gregory  
**Subject:** RE: MCHM & PPH Product TICs

I sent some comments to Steve and Matthew that may or may not be helpful to you.

Regarding methanol in crude MCHM as possible source of formaldehyde in DW:

Agree that oxidative degradation pathway of MCHM would be oxidation of the primary alcohol (attached to a carbon with 2 Hs) to an aldehyde (4-methyl cyclohexane -1-carbaldehyde, a chemical with a CAS but I cannot find information on its stability). Next oxidation of the aldehyde to a carboxylic acid.

I have read that MCHM is a byproduct of 1,4-cyclohexanedimethanol synthesis (CHDM). The other components of the crude MCHM appear to be oxidation products of MCHM or CHDM. Carboxylate (5% of crude), ether (methoxymethyl, 4-22%) and dicarboxylate (dimethyl ester, 1%).

If methanol is in the crude as stated in the Eastman MSDS, then it was likely added and not a byproduct or oxidative degradation product of MCHM. With the other big component in Crude MCHM being the 4-methoxymethylcyclohexane methanol (4-22%) maybe look how the ether linkage fragments in MS.

**Ex. 5 - Deliberative**

## **Ex. 5 - Deliberative**

and note,

FYI, just looked at description of patent process for making CHDM. It actually involves hydrogenation (reduction) of the dimethyl,1,4-cyclohexanedicarboxylate (1% of crude). So it's presence (dimethyl,1,4-cyclohexanedicarboxylate) in MCHM crude may be as unreacted starting material.

Point is, there is no methanol in synthesis of MCHM or CHDM.

Elizabeth

**From:** Gray, Wendy

**Sent:** Monday, February 03, 2014 11:56 AM

**To:** Magnuson, Matthew; Weber, Eric; Allgeier, Steve; Hedrick, Elizabeth; Arguto, William

**Cc:** Sayles, Gregory

**Subject:** RE: MCHM & PPH Product TICs

Matt,

The list that you have would be our preliminary list of chemicals in the tank with the exception that there was one more unknown identified by the VOC analysis:

Unknown, masses, masses 79, 94, 55 and 67

I think that there are really two questions that need to be answered.

- 1) What are potential TICs associated with chlorine disinfection of the list of preliminary chemicals in the tank?
- 2) Description of formaldehyde, reasons that it may have been found in drinking water, and likelihood of formation as byproduct of disinfection.

## Ex. 5 - Deliberative

I am going to tentatively set a call for tomorrow afternoon (first available time to collectively gather this distribution list), but there is a briefing tomorrow morning that may or may not make this discussion necessary/relevant.

Thanks!

Wendy Gray, P.E.  
Environmental Engineer  
US EPA Region III  
Drinking Water Branch  
1650 Arch Street (3WP21)  
Philadelphia, PA 19103  
Office: (215) 814-5673

Cell: (267) 216-6521  
Fax: (215) 814-2302  
[Gray.Wendy@EPA.gov](mailto:Gray.Wendy@EPA.gov)

**From:** Magnuson, Matthew  
**Sent:** Monday, February 03, 2014 11:10 AM  
**To:** Weber, Eric; Gray, Wendy; Allgeier, Steve; Hedrick, Elizabeth; Arguto, William  
**Cc:** Sayles, Gregory  
**Subject:** RE: MCHM & PPH Product TICs

Wendy,

# Ex. 5 - Deliberative

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The situation is further complicated by not knowing what that tank has been used for over the years, or even recently. We didn't even know about the PPH for a while.

# Ex. 5 - Deliberative

Thanks.

Matthew

<u>Compound</u>	<u>CAS number</u>	<u>MSDS</u>
Cyclohexanemethanol	100-49-2	Eastman
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	Eastman
Cyclohexanemethanol, 4-methyl-, cis-	????	Eastman

Cyclohexanecarboxylic acid, 4-methyl-, methyl ester	51181-40-9	Eastman
1-phenoxypropan-2-ol (PPH) (propylene glycol phenyl ether)	770-35-4	Dow
Possible 1,4-cyclohexanedimethanol	105-08-8	Eastman
A compound similar to Ethanol, 2-(4-methylphenoxy)-	NA	Dow?
1,4-Cyclohexanedicarboxylic acid, dimethyl ester (Dimethyl 1,4-cyclohexane dicarboxylate)	94-60-0	Eastman
Dipropylene glycol phenyl ether (4 peaks)	51730-94-0	Dow
Unknown, masses 108, 107 and 166	NA	
Unknown, masses 121, 59, 91 and 134	NA	
Unknown alcohol, masses 59, 135 and 107	NA	
Unknown alcohol, masses 59, 135 and 94	NA	
Unknown alcohol, masses 59, 135 and 107	NA	
Unknown alcohol, masses 59, 135 and 107	NA	
Unknown, masses 59, 135, 107 and 161	NA	

- Eastman = Eastman MSDS for Crude MCHM 10-19-05
- Dow = DOW MSDS for PPH, Basic, 11-15-11

**From:** Weber, Eric  
**Sent:** Monday, February 03, 2014 10:02 AM  
**To:** Gray, Wendy; Allgeier, Steve; Magnuson, Matthew; Hedrick, Elizabeth; Arguto, William  
**Subject:** RE: MCHM & PPH Product TICs

Wendy,

I should be able to get the list of chemicals thought to be in the tank out perhaps this afternoon, more likely tomorrow morning.

Eric

**From:** Gray, Wendy  
**Sent:** Monday, February 03, 2014 9:39 AM  
**To:** Weber, Eric; Allgeier, Steve; Magnuson, Matthew; Hedrick, Elizabeth; Arguto, William  
**Subject:** MCHM & PPH Product TICs

Good morning,

Just wanted to check in primarily with Matt and Eric, to see how we are coming along with possible tentatively identified compounds associated with the contaminants related to the incident?

Thanks for your help!

Wendy Gray, P.E.  
Environmental Engineer  
US EPA Region III

Drinking Water Branch  
1650 Arch Street (3WP21)  
Philadelphia, PA 19103  
Office: (215) 814-5673

Cell: (267) 216-6521  
Fax: (215) 814-2302  
[Gray.Wendy@EPA.gov](mailto:Gray.Wendy@EPA.gov)